

Master Thesis

Multi Phase Modelling an Finite Element Implementation of Steel Heat Treatment

conducted at

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by

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Chapter 1

Introduction

Heat treatment of metals as a way of altering its properties and microstructure is a process known for millennia. For many millennia heat treatment of metals has been an important part of industrial development. The ancient egyptians used annealing to

The heat treatment process of steel usually involves vigorously heating the metal and throwing it into cold water. A later less vigorous reheating is optional. *Maybe spare this for the presentation*

Define heat treatment

talk about history islamic, egypt, india, china, 9000 years bc

Chapter 2

Model/Theoretical Framework/Method

Heat treatment problems require the solution of three problems. Heat transfer, mechanical material response and phase transformation are coupled by their physical interactions.

2.1 Phase Transformations

Within this work two different kind of phase transformations are treated. Martensite transformation is athermal without thermal activation while the transformation into bainite is diffusion controlled. The bainite transformation is time dependent while martensite transformation is only driven by cooling, c.f. [Totten \[2007\]](#).

For the microstructural problem two different widely accepted (sources!!!) phenomenological models are used.

The martensitic transformation relies on the Koistinen-Marburger model established by [Koistinen and Marburger \[1959\]](#). It describes the transformation using the following equation

As dargelegt in the previous chapter athermal and diffusion-controlled phase transformations are treated in this thesis. In athermal transformations there is no thermal activation, e. g. incubation time and no time dependence. The transformation is purely driven by cooling. If there is no further cooling the transformation stops. The transformation from austenite to martensite is regarded as being athermal. It's modelling relies on the Koistinen-Marburger model established in [Koistinen and Marburger \[1959\]](#). It describes the evolution of the volume fraction of martensite β_M that is also depicted in fig. [2.1](#) using the following equation

$$\beta_M = 1 - e^{-k(M_S - T)} \quad . \quad (2.1)$$

The parameter k is material specific and describes the speed of the transformation. The martensite starting temperature M_S depends on the material and the other factors as the local carbon content that can be influenced by other phase transformations ??.. It determines the temperature at which the transformation starts. The transformation is

regarded as complete when the martensitic volume fraction reaches 99%. The martensite finish temperature M_F can be calculated by rearranging 2.1 and inserting $\beta_M = 99\%$.

The rate of the martensitic transformation can be described by

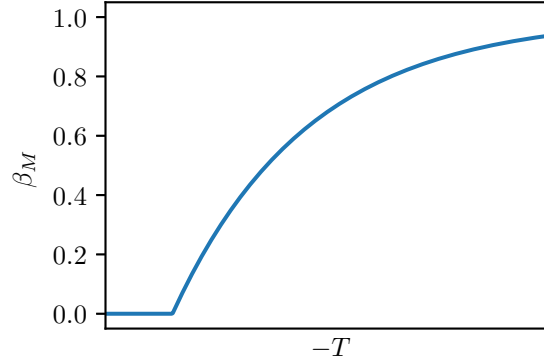


Figure 2.1: Development of the martensite volume fraction under cooling.

$$\dot{\beta}_M = -e^{-k[M_S - T]} k \dot{T} = \left[1 - e^{-k[M_S - T]} - 1 \right] k \dot{T} = -[1 - \beta_M] k \dot{T} \quad . \quad (2.2)$$

While this equation is valid when only considering the transformation from austenite to martensite it can be generalized for the usage with more phase transformations by interpreting the term $1 - \beta_M$ as the remaining austenite β_A available for transformation. This yields the following rate for the evolution of the martensitic phase

$$\dot{\beta}_M = -\beta_A k \dot{T} \quad . \quad (2.3)$$

The other transformation considered in this thesis is regarded as diffusion-controlled with thermal activation. There is a time-dependence in these transformations and they do continue isothermally when the cooling is stopped ??.. The transformation from austenite to bainite falls into this category. Schlecht.

Diffusional processes and transformations are often modelled using the... The equation used to describe this transformation is the JMAK law developed by Johnson, Mehl, Avrami and Kolmogorov (Avrami, 1940; Cahn, 1956) which is only valid for isothermal transformations. The JMAK law

$$\beta_B = \hat{\beta}_B [1 - e^{-b_B (t^{N_B})}] \quad (2.4)$$

can be used for various diffusional transformations and other time dependent processes Here it is used to model the development of the volume fraction of bainite β_B where $\hat{\beta}_B$ is the maximal amount of bainite reached in the transformation. Irgendwas mit $\hat{\beta}_B = \beta_A + \beta_B$

with the maximal volume fraction of bainite $\hat{\beta}_B = \beta_A + \beta_B$ that can be reached if all austenite and the yields sigmoidal shapes seen in fig. 2.3 with a slow start and a slow finish of the transformation but a high rate in between. The parameters

$$N_B(T) = \frac{6.1273}{\ln\left(\frac{t_B^f}{t_B^s}\right)} \quad \text{and} \quad b_B(T) = \frac{0.01005}{(t_B^s)^{N_B(T)}} \quad (2.5)$$

are derived using the starting and finishing time t_B^s and t_B^f for the diffusive transformation. Those are defined at volume fraction of 1% and 99% of the target phase. The parameters are temperature dependent and can be determined from experimental TTT diagrams (Diss Yu 1977 oder so).

The time derivation of the JMAK law eq. 2.4 yields the rate equation for isothermal cooling

$$\dot{\beta}_B = \hat{\beta}_B b_B N_B t^{(N_B-1)} [1 - \beta_B] \quad . \quad (2.6)$$

As the JMAK law—and TTT-diagrams from which the parameters are derived—is only valid for isothermal transformations it has to be adapted to depict a cooling process.

In Scheil [1935] a theory of the additivity of fractional nucleation is developed to predict the start of transformation from austenite during cooling. The so-called ‘additivity rule’ states that transformation starts when the fractions of nucleation $\frac{\Delta t_i}{\tau(T_i)}$ amassed during the cooling reaches unity.

$$\int_{T_0}^{T_x} \frac{dt}{\tau(T)} = 1 \quad (2.7)$$

where T_0 is an equilibrium temperature at which no nucleation happens, T_x is the temperature at which the transformation starts when following an anisothermal temperature path and $\tau(T)$ is the incubation time after that transformation starts for an isothermal temperature path. This means for a discretized calculation that the transformation starts when the fractions of nucleation at every time increment $\frac{\Delta t_i}{\tau(T_i)}$ amassed during the cooling reaches unity as follows

$$\sum \frac{\Delta t_i}{\tau(T_i)} = 1 \quad . \quad (2.8)$$

It is shown in Lusk and Jou [1997] and Christian [2002] that this holds true for transformations that are isokinetic, c.f. Cahn [1956], and whose rate can be expressed in the following form

$$\dot{\beta} = h(\beta)g(T) \quad (2.9)$$

like eq. 2.6.

Based on the additivity rule Tzitzelkov et al. [1974] developed an algorithm to predict the phase development for continuous cooling. For this the cooling cure A continuous temperature curve can be discretized into isothermal increments as in fig. 2.2.

The cooling curve is discretized into small isothermal steps at declining temperatures. Every step i is defined by it’s temperature T_i and it’s duration Δt_i .

In the following the procedure is explained using two isothermal steps of $\Delta t = 1.5s$ at the temperatures $T1 = 600^\circ C$ and $T2 = 550^\circ C$.

The first step starts at P0 with a volume fraction of bainite $\beta_B = 0$ and ends at P1 after Δt at $\beta_B^1 = 0.17$ following the transformation curve for T1. For the next step at T2, a fictitious point P1* is introduced. It is the intersection of $\beta_B = \beta_B^1$ with the transformation curve for T2. The time will be called fictitious time t^* . It is the time transformation at T2 would take to yield β_B^1 .

Then transformation is again following the curve for T2 for a Δt of 1.5s finishing at a volume fraction β_B of 0.78.

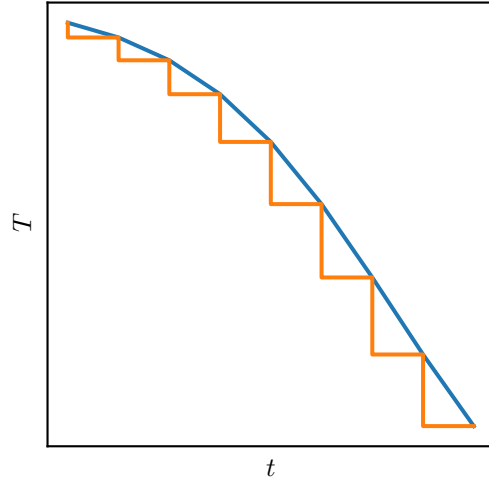


Figure 2.2: Continuous and incrementally isothermal discretized cooling curve.

To incorporate the fictitious time into the rate equation the steps laid out in (Reti 2001) are done. Using the JMAK law 2.4, the fictitious time for a given volume fraction β_B and a temperature T the fictitious time t^* is derived as

$$t^* = \left(\frac{\ln A}{b(T_{i+1})} \right)^{\frac{1}{N(T_{i+1})}}, \quad A = \frac{\hat{\beta}}{\hat{\beta} - \beta_i} \quad . \quad (2.10)$$

This relation then is inserted into the rate equation 2.6 to replace the isothermal transformation time and eliminate the explicit time dependence

$$\dot{\beta} = N b^{\frac{1}{N}} (\hat{\beta} - \beta) (\ln A)^{1 - \frac{1}{N}} \quad . \quad (2.11)$$

The generalization of the rate equation for more phases *works similar* to the generalization of the martensitic rate. The maximal volume fraction of bainite $\hat{\beta}$ in (Oliviera 2010) is interpreted as

$$\hat{\beta} = \beta_A + \beta_B = 1 - \beta_M \quad . \quad (2.12)$$

This leads to a desired coupling of the rate equations of Bainite and Martensite.

2.1.1 Involved Phases

Floris Osmond named Martensite after Adolf Martens in [Osmond \[1904\]](#)

2.1.2 phenomenological models

Kostinen Marburg

JMAK

Bringe ich die Metallurgie in dieses Kapitel und mische sie mit den Gleichungen oder trenne ich es in zwei Kapitel?

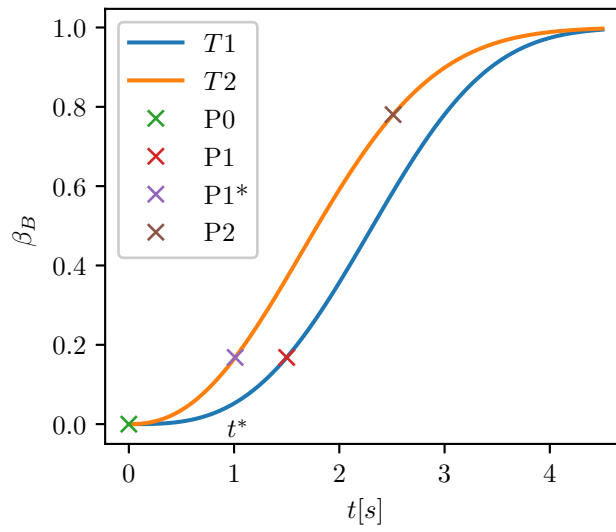


Figure 2.3: Two isothermal cooling steps.

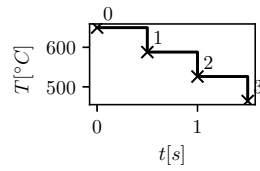


Figure 2.4: Discretized example cooling curve.

2.2 Thermal Problem

The thermal problem is governed by the heat equation

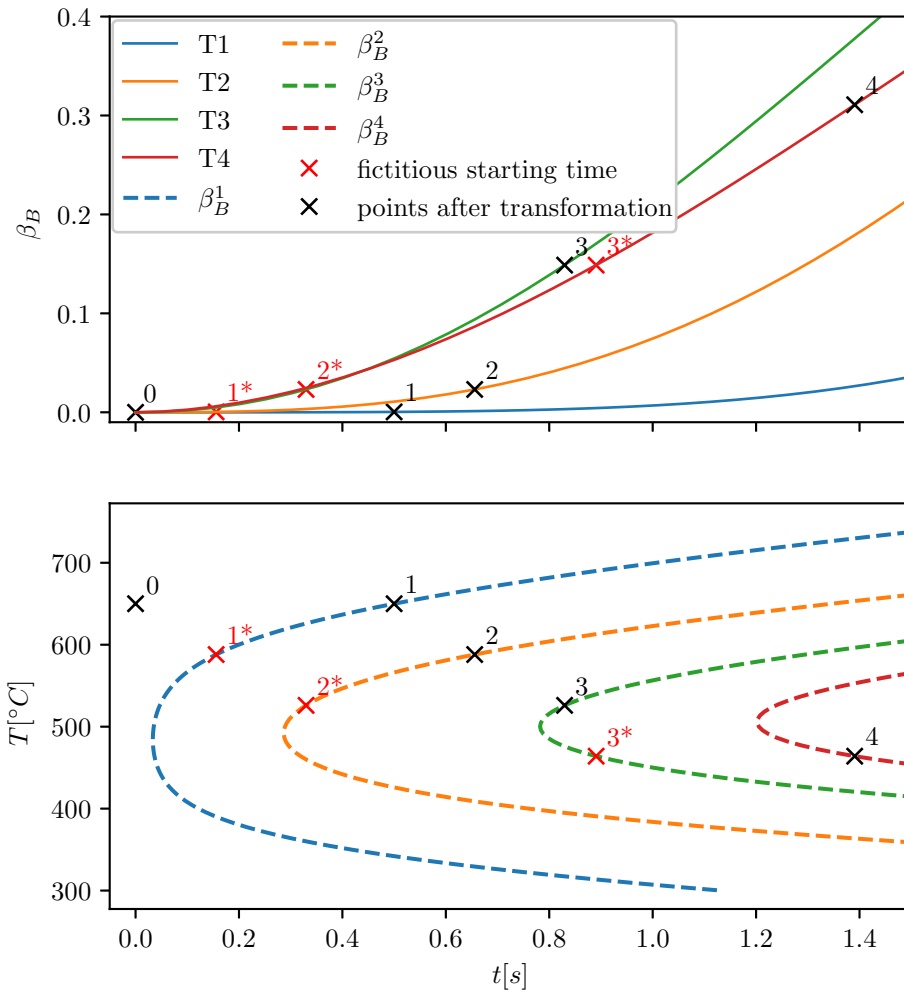


Figure 2.5:

Chapter 3

Algorithmic implementation

After establishing the rate equations for the phase transformations 2.11 and 2.3 in the previous chapter 2 there are modifications and regularisations necessary before one is able to use them for computation. For both equations a term ζ is introduced that controls whether transformation is happening or not, cf. Pacheco et al. [2001] and de Oliveira et al. [2010].

For the martensitic transformation $\zeta_{A \rightarrow B}$ contains two heaviside functions Γ and a regularized step function using a tanh. The first heaviside function $\Gamma(-\Delta T)$ ensures irreversibility and that transformation only occurs during cooling. The second heaviside function $\Gamma(T - M_F)$ prevents transformation below the martensite finish temperature. The regularized step function $\tanh(A(M_S - T))/2 + 1/2$ starts the transformation after the temperature is below the martensite starting temperature. The regularization deals with the discontinuity of the transformation rate at $T = M_S$. The influence of A is depicted in fig. 3.1. The choice of $A = 1$ makes the effect of the regularization disappear

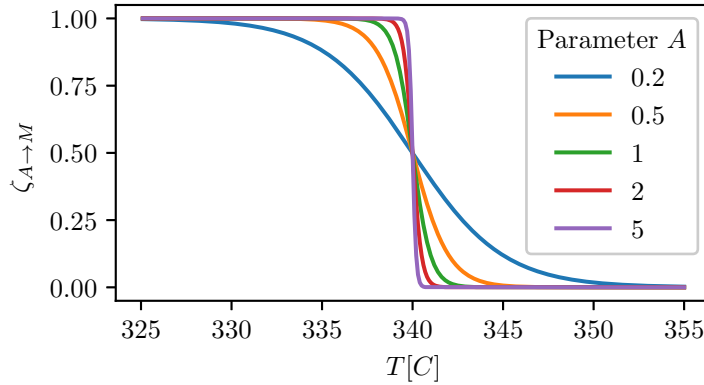


Figure 3.1: Regularized step function using a tanh with different parameters.

($< 1e - 6$) at $M_S \pm 2\%$.

This yields the extended rate equation for the evolution of the martensitic volume fraction

$$\dot{\beta}_M = -\zeta_{A \rightarrow M} \beta_A k \dot{T} \quad (3.1)$$

$$\text{with } \zeta_{A \rightarrow M} = \Gamma(-\Delta T) \Gamma(T - M_F) (\tanh(A(M_S - T))/2 + 1/2) \quad (3.2)$$

For the bainite transformation a new local time scale for every material point is

introduced. The transformation time τ starts once the temperature at the material point drops below the bainite starting temperature T_B^s . This time scale is used to account for vastly different incubation times at different temperatures. The incubation time is regarded as the time on the left of the bainite starting time t_B^s when looking at the TTT Diagram in fig. ??..

The time on the left of the bainite starting time t_B^s when looking at the TTT Diagram in fig. ??.. is regarded as incubation time. The incubation time τ necessary to start the transformation is vastly different at different temperatures. To account for this in a similar way to the anisothermal evolution of bainite, Scheill's additivity ?.. is used to determine when t_B^s is reached following a cooling curve.

The following condition is checked at every time step after an update of τ to determine the start of the transformation

$$\tau = \tau + \frac{\Delta T}{t_B^s} \quad (3.3)$$

$$t_B^s \geq \tau \quad . \quad (3.4)$$

The initial value problem represented by the rate equations is solved by implicit time integration which leads to the evolution equation $\beta^{n+1} = \beta^n + \Delta\beta^{n+1}$, with $\Delta\beta^{n+1} = \Delta t \dot{\beta}^{n+1}$.

After bringing these equations into residual form

$$\begin{aligned} \underline{\mathbf{R}}_\beta &= \underline{\beta}^{n+1} - \underline{\beta}^n - \underline{\Delta\beta} \\ &= \begin{bmatrix} R_{\beta_B} \\ R_{\beta_M} \end{bmatrix} = \begin{bmatrix} \beta_B^{n+1} - \beta_B^n - \Delta\beta_B^{n+1} \\ \beta_M^{n+1} - \beta_M^n - \Delta\beta_M^{n+1} \end{bmatrix} \end{aligned} \quad (3.5)$$

$$\text{with } \underline{\Delta\beta} = f(\underline{\beta}^{n+1}) \quad (3.6)$$

the backward Newton method is used to solve the equation system 3.5. The update of the backward Newton

$$\underline{\beta}^{k+1} = \underline{\beta}^k - \frac{\underline{\mathbf{R}}_\beta}{\underline{\mathbf{R}}_{\beta'}} \quad (3.7)$$

with the iteration counter k requires the derivation of the tangent

$$\underline{\mathbf{R}}_{\beta'} = \begin{bmatrix} \frac{\partial R_{\beta_B}}{\partial \beta_B} & \frac{\partial R_{\beta_B}}{\partial \beta_M} \\ \frac{\partial R_{\beta_M}}{\partial \beta_B} & \frac{\partial R_{\beta_M}}{\partial \beta_M} \end{bmatrix} \text{ with} \quad (3.8)$$

$$\frac{\partial R_{\beta_B}}{\partial \beta_B} = 1 - \Delta t b^{\frac{1}{N}} N \left[B^{1-\frac{1}{N}} - \left(1 - \frac{1}{N}\right) B^{-\frac{1}{N}} \right] \quad (3.9)$$

$$\frac{\partial R_{\beta_B}}{\partial \beta_M} = -\Delta t b^{\frac{1}{N}} N \left[B^{1-\frac{1}{N}} - \left(1 - \frac{1}{N}\right) B^{-\frac{1}{N}} \left(1 - \frac{\beta_A}{1 - \beta_M}\right) \right] \quad (3.10)$$

$$\frac{\partial R_{\beta_M}}{\partial \beta_B} = -k \Delta T \zeta_{A \rightarrow M} \quad (3.11)$$

$$\frac{\partial R_{\beta_M}}{\partial \beta_M} = 1 - k \Delta T \zeta_{A \rightarrow M} \quad . \quad (3.12)$$

Bibliography

- Cahn, J. W. (1956). Transformation kinetics during continuous cooling. *Acta Metallurgica*, 4(6):572–575.
- Christian, J. (2002). Formal Theory of Transformation Kinetics. In *The Theory of Transformations in Metals and Alloys*, pages 529–552. Elsevier.
- de Oliveira, W. P., Savi, M. A., Pacheco, P. M. C. L., and de Souza, L. F. G. (2010). Thermomechanical analysis of steel cylinders quenching using a constitutive model with diffusional and non-diffusional phase transformations. *Mechanics of Materials*, 42(1):31–43. Number: 1.
- Koistinen, D. and Marburger, R. (1959). A general equation prescribing the extent of the austenite-martensite transformation in pure iron-carbon alloys and plain carbon steels. *Acta Metallurgica*, 7(1):59–60. Number: 1.
- Lusk, M. and Jou, H.-J. (1997). On the rule of additivity in phase transformation kinetics. *Metallurgical and Materials Transactions A*, 28(2):287–291.
- Osmond, F. (1904). *Microscopic Analysis of Metals*. Charles Griffin & Company, Limited, London.
- Pacheco, P. M. C. L., Savi, M. A., and Camarão, A. F. (2001). Analysis of residual stresses generated by progressive induction hardening of steel cylinders. *The Journal of Strain Analysis for Engineering Design*, 36(5):507–516. Number: 5.
- Scheil, E. (1935). Anlaufzeit der Austenitumwandlung. *Archiv für das Eisenhüttenwesen*, 8(12):565–567.
- Totten, G. E., editor (2007). *Steel heat treatment handbook*. CRC, Taylor & Francis, Boca Raton.
- Tzitzelkov, I., Hougardy, H. P., and Rose, A. (1974). Mathematische Beschreibung des Zeit-Temperatur-Umwandlung-Schaubildes für isothermische Umwandlung und kontinuierliche Abkühlung. *Archiv für das Eisenhüttenwesen*, 45(8):525–532.